Biophysical Chemistry 6582 Exam 1 MARCH 1, 2004,

I will not cheat today, signed _____ print name: KEY

1. (25) Consider a two-dimensional unit cell with a axis = 100 and b axis = 100, with gamma = 90,

(a) sketch the cell, and add the 3 2 planes,

(b) in (a) illustrate Braggs law, sketch two incoming and outgoing rays, indicate the angle theta, the d-spacing and the path difference,



(no calculations are required to answer c-h, circle the correct response)

(c) would the d-spacing for the 3 3 planes be

less than, greater than, or equal to the d-spacing for the 4 4 planes? [comment: increasing h and k decreases the spacing] (d) would the d-spacing for the 3 3 planes be less than, greater than, or equal to the d-spacing for the 2.3 planes? [decreasing either h or k alone increases the spacing] (e) would the d-spacing for the 3 3 planes be less than, greater than, or equal to the d-spacing for the 3 2 planes? (f) would the angle theta for the 3 3 planes be less than, greater than, or equal to the angle theta for the 4 4 planes? [increasing the d spacing decreases θ (n λ =2dsin θ)] (g) would the angle theta for the 3 3 planes be less than, greater than, or equal to the angle theta for the 2 3 planes? (h) would the angle theta for the 3 3 planes be less than, greater than, or equal to the angle theta for the 3 2 planes?

2) (25) Indicate the point symmetry (not necessarily the point group) of the following molecules (draw the molecule and the symmetry operators:

a) Water (H_2O)

A twofold bisects the H-O-H bonds. One mirror is in the plane of the three atoms H, O, H. A second mirror is perpendicular to first, and contains the twofold axis.

b) Carbon tetrachloride (CCl₄)

There are threefolds along each C-Cl bond. Twofolds bisect each pair of C-Cl bonds There are mirrors in the plane of each set of Cl-C-Cl.

c) CIFClBr (Carbon bonded with 4 different kinds of halogen atoms)

No symmetry at all.

3) (25) For the questions below:

(For full credit, the c-displacement indicators must be equal to or less than 0, and equal to or less than 1) (a) Sketch a 6_1 screw axis (viewing down the screw axis, i.e., the c-axis) with all the equivalent positions.



(b) Sketch a 6_4 screw axis (viewing down the axis) with all the equivalent positions.





4) (25) Add the equivalent positions to the symmetry elements below.